

Polarization as a topological quantum number in graphene

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Graphene, with its quantum Hall topological (Chern) number reflecting the massless Dirac particle, is shown to harbor yet another topological quantum number. This is obtained by combining Středa's general formula for the polarization associated with a second topological number in the Diophantine equation for the Hofstadter problem, and the adiabatic continuity, earlier shown to exist between the square and honeycomb lattices by Hatsugai et al. Specifically, we can regard, from the adiabatic continuity, graphene as a “simulator” of square lattice with half flux quantum per unit cell, which implies that the polarization topological numbers in graphene in weak magnetic fields is $1/2$ per Dirac cone for the energy region between the van Hove singularities, signifying a new quantum number characterizing graphene.

Introduction— Characterization of quantum states with topological numbers appears in various phenomenon in condensed-matter physics[1–7]. Topologically non-trivial states are characterized by nonzero topological numbers, which replace the order parameters in systems characterized by spontaneous symmetry breaking. A canonical model is the quantum Hall effect (QHE) with the Chern number characterizing the topological properties, where lattice structures (or periodic potentials) make the systematics of the topological numbers (known as Hofstadter's problem.[8]) versatile. The topological numbers in this problem are determined by a Diophantine equation, the so-called TKNN formula[1], which was also obtained by the Widom-Středa formula[9, 10]. Hofstadter's problem has been examined not only in condensed-matter systems but recently also in cold-atom systems with greater experimental controllability[11, 12]. A correspondence between bulk and edge topological properties (bulk-edge correspondence[13]) in the Hofstadter problem has in fact been confirmed in cold-atom systems[14]. Lattice structure exerts an unusual effect on topological numbers, where a canonical example is honeycomb lattice as in graphene, where a QHE specific to massless Dirac particles appears[15–18], indicating that topological numbers can be dramatically affected by the lattice structure.

Now, in the Diophantine equation, there exists actually a *second topological number*, which has long been known but its physical meaning was revealed only recently by Středa and coworkers, where the second topological number is shown to represent an electric polarization[19–21]. These (i.e., graphene QHE and polarization quantum numbers) have motivated us to look into the following question: Does graphene harbor another topological number peculiar to a massless Dirac system besides the

QHE number? We shall show that there exists indeed an intriguing polarization quantum number in graphene. To derive this we have fully exploited an *adiabatic continuity between the topological numbers for square and honeycomb lattices* as Hatsugai and coworkers have earlier shown[17], with which we can obtain a correspondence between the topological numbers for the two lattices. With this we can obtain Středa's polarization topological numbers in graphene. An intriguing starting point is that the adiabatic continuity implies that graphene is a “half-flux simulator” (an adiabatic realization of square lattice with half flux quantum per unit cell), whose consequence is that the polarization topological number in graphene in weak magnetic fields is $1/2$ for a wide energy region (that encompasses the two van Hove singularities). Thus this provides a novel topological quantum number characterizing graphene.

Diophantine equation and topological numbers— Let us start with the Hofstadter problem, i.e., non-interacting fermions in a two-dimensional, periodic lattice or potential in a uniform magnetic field, for which the Hamiltonian in the tight-binding case reads $H = -\sum_{ij} e^{i\theta_{ij}} c_i^\dagger c_j$, where we have taken the transfer energy as the unit of energy, and the Peierls phase θ_{ij} takes care of the magnetic flux $\phi = (2\pi)^{-1} \sum_{ij} \theta_{ij}$ per unit cell in units of the flux quantum $\Phi_0 \equiv h/e$. If we vary $\phi = p/q$ over rational values with (p, q) mutually prime integers, we have a fractal energy spectrum (Hofstadter's butterfly). The Diophantine equation for the topological quantum numbers[1] is

$$r = t_r p + s_r q \equiv t_r p \pmod{q}, \quad (1)$$

where r labels the energy gaps from below, t_r is the QHE topological (Chern) number, while s_r is the number in question. For a given set of values of (r, p, q) a pair of integers (t_r, s_r) can be determined. For a square lattice with nearest-neighbor hopping, the Diophantine equation has a unique solution if one imposes $|t_r| \leq q/2$. This constraint is perturbatively justified with an adiabatic argument. It is rather surprising that the integer

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t_r , which is determined by an algebraic (i.e. Diophantine) equation should coincide with a differential geometrical (topological Chern) number, as confirmed by the Widom-Středa argument[9, 10]. The formula shows, via a Maxwell relation, that $\sigma_{yx} = e(\partial n/\partial B) = (\partial \rho/\partial B)$, where $n = N/A$ is the density of electron with N the total number and A the total area of the system. With $\phi = A_0 B/\Phi_0$, $r/q = nA_0$, where $A_0 = a^2$ is the area of a unit cell, we have $\partial(r/q)/\partial \phi = (e/h)(\partial n/\partial B)$, which reads, when combined with the Diophantine equation, $r/q = t_r \phi + s_r$,

$$\sigma_{yx} = e \frac{\partial n}{\partial B} = \frac{e^2}{h} t_r,$$

i.e., t_r exactly coincides with the Chern number.

The Diophantine equation reads in the original units as

$$n = \left(\frac{\sigma_{yx}}{e^2/h} \right) \left(\frac{B}{h/e} \right) + \frac{s_r}{A_0}, \quad (2)$$

or

$$\rho' \equiv \rho - \delta \rho = \sigma_{yx} B, \quad (3)$$

where $\rho \equiv en$ is the charge density, and $\delta \rho \equiv (e/A_0)s_r$. Středa and coworkers have shown that $\delta \rho \propto s_r$ is the electric polarization induced by the magnetic field as a quantum effect.[19–22] Indeed, Eq.(2) is expressed as $\frac{1}{A} \frac{\partial N}{\partial A_0} |_B = -(s_r/A_0^2)$, which is just Eq.(14) in [22].

Physically, the Lorentz force acting on a particle of velocity v_y is compensated by the induced electric field E_x in Laughlin's cylindrical geometry. The condition for the balance is $ev_y B = eE_x$. We can then express the Hall current as a flow of the “screened” charge density, $\rho' = \rho - \delta \rho$, as $I_y/L_x = \rho' v_y$, $V_x/L_x = E_x$, where L_x is the width of the cylinder and V_x the Hall voltage. Then the Hall conductivity is written as

$$\sigma_{yx} = \frac{I_y}{V_x} = \frac{\rho' v_y}{E_x} = \frac{\rho'}{B},$$

which indeed implies $\rho' = \sigma_{yx} B$, as consistent with the Diophantine Eq.(3).

Semiclassics around rational fluxes— Before addressing the adiabatic continuity, we need to look at the semiclassical behavior around rational fluxes for the polarization s_r . For the square lattice with the nearest-neighbor hopping, the Hofstadter's butterfly is as in Fig.2, right panel, and the Chern number is given by the t_r with $|t_r| \leq q/2$. There is relatively a large gap for each simple fraction P/Q , and in its vicinity the semiclassical approximation should be appropriate, so let us examine the polarization there. For this purpose one may define a reduced magnetic flux $\Delta \phi$ as a small deviation from a simple flux $\Phi = P/Q$ as $\phi = p/q = P/Q + \Delta \phi$. We can then regard the Hofstadter problem at ϕ as composed of the *effective* Landau levels formed by the reduced magnetic flux $\Delta \phi$. The reduced magnetic field is naturally defined

as $\tilde{B} \equiv (\Phi_0 \Delta \phi)/A_0$, which implies, with the Diophantine equation (3) in the original units, that the reduced polarization $\delta \tilde{\rho}$ is

$$\rho = \sigma_{yx} B + \delta \rho \equiv \sigma_{yx} \tilde{B} + \delta \tilde{\rho}.$$

This defines the reduced polarization quantum number,

$$\begin{aligned} \tilde{s}_r &\equiv \left(\frac{A_0}{e} \right) \delta \tilde{\rho} = s_r + \sigma_{yx} \left(\frac{\Phi_0}{e} \frac{P}{Q} \right) \\ &= s_r + t_r \frac{P}{Q} = \frac{r}{q} - t_r \Delta \phi, \end{aligned} \quad (4)$$

where we have used Eq.(1).

We can illustrate this for three cases, $\Phi = 0, 1/2$ and 1. Near $\Phi = 0$, the standard Landau levels for a two-dimensional electron gas are realized for $\phi = 1/q$. For the less than half-filled case (electron side; $r < q/2$), we have $t_r = r$, which trivially implies $\tilde{s}_r = s_r = (A_0/e)\delta \rho = 0$. On the hole side ($r > q/2$) the solution of the Diophantine equation is given by $t_r = q - r$, which implies $\tilde{s}_r = s_r = (A_0/e)\delta \rho = 1$. Namely, \tilde{s}_r against the Fermi energy E_F is given as $\tilde{s}(E_F) = 0 (E_F < 0), 1 (E_F > 0)$, where \tilde{s}_r is specified by the Fermi energy E_F in the r -th gap as $\tilde{s}(E_F) = \tilde{s}_r$ [23]. Hence $\tilde{s}(E_F)$ is a simple step function with the step situated at $E = 0$, square lattice's van Hove singularity in the band dispersion in zero magnetic field. A numerical result for weak magnetic fields is shown in Fig.1, which confirms the analytical arguments. Near $\Phi = 1$, with $\phi = (q-1)/q$ ($\Delta \phi = -1/q$), we can show that \tilde{s}_r is given by the same function as in the above case for near $\Phi = 0$, which is consistent with the periodicity of the Hofstadter problem. Note that the original s_r itself does not satisfy this periodicity, which implies the reduced polarization $\delta \tilde{\rho}$ is more physical.

Now we come to the case in question, $\Phi = 1/2$ (π -flux). As shown in [17], if we want to adiabatically relate a honeycomb lattice with a flux $1/q'$ to a square lattice, we can consider a square lattice with a flux $\Delta \phi = 1/2q'$ on top of π flux per unit cell, i.e.,

$$\phi = \frac{p}{q} = \frac{1}{2} + \Delta \phi = \frac{q' + 1}{2q'},$$

where $q' + 1$ is assumed to be prime with $2q'$. As shown in [17], every step in the Chern number t_r against E_F has a height of 2 everywhere except at the van Hove singularities of the π -flux band at $\pm 2\sqrt{2}$. The energy spectrum of the Hofstadter problem in the $\Delta \phi \rightarrow 0$ limit is composed of touching two bands (see Fig.2). Then near the band bottom of the π -flux bands below the van Hove energy $-2\sqrt{2}$, we can put $r = 2r'$ ($r' = 1, 2, \dots, q'/2$), for which the Diophantine equation, $2r' \equiv (q' + 1)t_{2r'} \pmod{2q'}$, $|t_{2r'}| < q'$, has a solution $t_{2r'} = 2r'$, which implies $s_{2r'} = [2r' - t_{2r'}(q' + 1)]/2q' = -r'$. Then the reduced polarization quantum number is trivially $\tilde{s}_{2r'} = -r' + 2r'(1/2) = 0$. If we turn to the r -th gap on the hole side above the van Hove energy at $2\sqrt{2}$, we can put $r = 2(q' - r')$, ($r' = 1, \dots, q'/2$), for which the Diophantine equation, $2(q' - r') \equiv (q' + 1)t_{2(q' - r')} \pmod{2q'}$

has a solution $t_{2(q'-r')} = -2r'$, giving $s_{2(q'-r')} = [2(q' - r') - t_{2(q'-r')}(q' + 1)]/2q' = r' + 1$, and the reduced polarization quantum number, $\tilde{s}_{2(q'-r')} = r' + 1 - 2r'(1/2) = 1$.

In the region of interest (for Dirac electrons residing between the van Hove singularities, $-2\sqrt{2} < E_F < 2\sqrt{2}$) it is convenient to introduce the usual Landau index, $N (= 0, \pm 1, \pm 2, \dots)$, with $N = 0$ corresponding to the level at $E = 0$. As depicted in Fig.2, there are $2q'$ Landau bands, since each level is composed of two (with a tiny gap not visible in Fig.2), so that we have $r = q' + 1 + 2N$ ($N = -q'/2, \dots, -1, 0, 1, \dots, q'/2 - 1$). The Diophantine equation,

$$q' + 1 + 2N \equiv t_r(q' + 1) \pmod{2q'}, \quad |t_r| < q'$$

then has a solution $t_r = 2(N + 1/2)$, which is the Chern number for the Dirac fermions with doubling. The polarization is $s_r = [r - (2N + 1)(q' + 1)]/2q' = -N$, and the reduced polarization quantum number becomes

$$\tilde{s}_r = -N + (2N + 1) \cdot \frac{1}{2} = \frac{1}{2}.$$

So we end up with a key result,

$$\tilde{s}(E_F) = \begin{cases} 0 & (E_F < -2\sqrt{2}) \\ \frac{1}{2} & (-2\sqrt{2} < E_F < 2\sqrt{2}) \\ 1 & (2\sqrt{2} < E_F) \end{cases} \quad (5)$$

In Fig.1(b) we have numerically calculated the Chern number t_r , the Středa's polarization s_r and the reduced polarization \tilde{s}_r against the Fermi energy for $\Phi = 1/2$. The result indeed confirms the analytical result, eq.(5).

We have also calculated t_r, s_r and \tilde{s}_r for a series of rational fluxes, e.g. for $\phi_0 = 1/5, 2/5$ etc, and the results are rather surprising in that the reduced polarization around a rational flux p/q is given quite simply as

$$\tilde{s}(E_F) = \frac{n}{q}, \quad E_{\text{vH}}^n < E_F < E_{\text{vH}}^{n+1}, \quad n = 0, 1, \dots, q \quad (6)$$

where E_{vH}^n is the energy of van Hove singularities in the n -th Hofstadter band from below. It signifies a *topological character of the reduced polarization quantum number* \tilde{s}_r in that only the (van Hove) singularities can change the sequence of \tilde{s}_r .

Graphene— In a honeycomb lattice in a flux $\phi_h = 1/q$ per hexagon, a finding in Ref.[17] is that the large gaps in graphene remain open in an adiabatic continuity between square and honeycomb lattices where the diagonal transfer t' for each hexagon is changed from 1 to 0. Further surprise is that this holds not only around the zero energy, but all the way up to the van Hove singularity, $E_{\text{vH}}^{1,2} \simeq \pm 1$, for honeycomb lattice. Since the adiabatic mapping between honeycomb and square lattices is given as

$$\begin{aligned} \text{honeycomb} : \phi_h &= 1/q \\ \leftrightarrow \text{square} : \phi_s &= 1/2 + \phi_h/2 = (q + 1)/2q, \end{aligned}$$

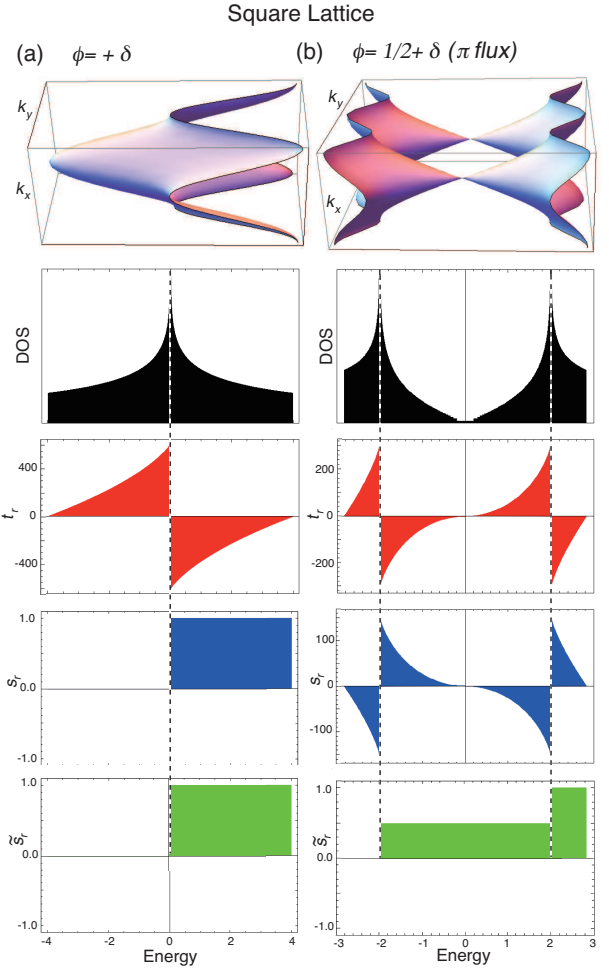


FIG. 1: For the square lattice, the band dispersion (with the energy as a horizontal axis), density of states $D(E)$, Chern number t_r , polarization topological number s_r and screened polarization \tilde{s}_r are plotted against energy for a small $\phi = \delta$ (left panel) or around the π flux, $\phi = 1/2 + \delta$ (right) with $\delta = 1/1223$. Small gaps are neglected. Dashed lines indicate van-Hove singularities.

i.e., a honeycomb lattice in weak magnetic fields translates into a square lattice around *half flux*, as depicted in Fig.2, we can directly apply the above result for the square lattice around half flux. We have only to note that, similar to the π flux case of the square lattice, the gap is rewritten in terms of the Landau index, N , this time for graphene Landau levels (with $N = 0$ labeling the level at $E = 0$), which is related to r as $r = q + 1 + 2N$. By the adiabatic continuity for the Chern number, we have $t_r = 2N + 1$, which reproduces the graphene QHE number as doubled Dirac cone contributions ($2(N + 1/2)$). Then the polarization quantum number is given as

$$s_r = 1.$$

Below the lower van Hove energy, the Hall conductance is simply $t_r = r$ ($r < q/2$), that is, $s_r = 0$. Above the upper

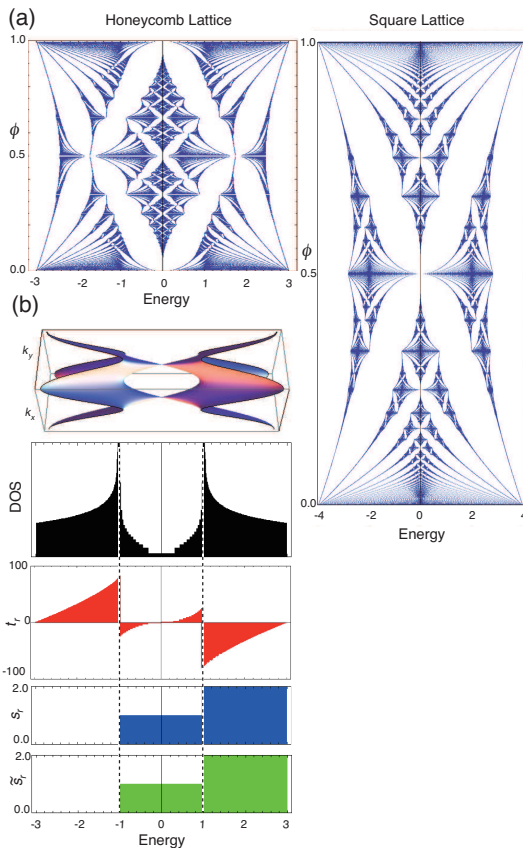


FIG. 2: (a) Hofstadter butterfly (one-particle energy spectrum vs magnetic field ϕ) for the tight-binding model for honeycomb (left panel) or for square (right) lattices. To indicate the correspondence, $1/q \leftrightarrow 1/2 + 1/2q$, between the two, energy scales are doubled with a shift by $1/2$. The butterfly for flux $\phi = p/q$ with all the prime $q \leq 179(1987)$ are plotted for honeycomb (square). Dashed line indicates the above correspondence. (b) For the honeycomb lattice, the band dispersion (with the energy as a horizontal axis), density of states $D(E)$, Chern number t_r , polarization topological number s_r and screened polarization \tilde{s}_r are plotted against energy for a weak $\phi = \delta (= 1/107)$. Small gaps are neglected. Dashed lines indicate van-Hove singularities.

van Hove energy, we have $t_r = -(2q - r)$ ($r > 3q/2$), which implies $s_r = 2$. Thus the polarization quantum number of the graphene against the Fermi energy is

$$s = \tilde{s} = \begin{cases} 0 & (E_F < E_{\text{vH}}^1) \\ 1 & (E_{\text{vH}}^1 < E_F < E_{\text{vH}}^2) \\ 2 & (E_{\text{vH}}^2 < E_F) \end{cases}$$

Namely, since the unit cell area in honeycomb is twice that in π -flux square lattice, \tilde{s} is doubled, which is consistent with the contribution of $1/2$ per Dirac cone. Thus graphene can indeed be considered as the “half-flux simulator” of the Hofstadter problem. This is the key result for graphene. We have numerically calculated the polarization in Fig.2 (bottom left panel), which confirms this formula. Since we take a weak magnetic field for graphene there, the reduced polarization coincides with the polarization itself ($\tilde{s}_r = s_r$).

In general, however, \tilde{s}_r and s_r can deviate from each other as in square lattice even for graphene. Near a generic rational flux $\phi_h = P/Q$, one can define the reduced polarization quantum number as $\tilde{s}_r = s_r + t_r(P/Q)$, which takes fractional values in general. For instance, the reduced polarization for graphene near the $1/2$ flux resembles the case for the square lattice near the $1/4$ flux (see the supplemental material).

To summarize, we have shown that graphene harbors, in addition to the quantum Hall topological number, another topological quantum number as the electric polarization. An interesting future problem is how to experimentally observe this, which may be possible if the electron density n is independently measures, since the other topological number has to do with the difference between $\sigma_{yx}B$ and $\rho = en$.

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